EXPERIMENT No. 1

Page No. 1 Date

- Spectral Identification No : 1

A] Preliminary Observation

I] IR Spectroscopy

Observation	Inference
a) Strong observation at 1724 cm^{-1}	C=O stretching i.e. acid, ketone, aldehyde may be present.
b) Medium observation in region 3100 - 2900 cm^{-1}	C-H stretching aryl/vinyl (sp^2) & alkyl C-H (sp^3) may be present.

II] ^1H NMR Spectroscopy

Observation	Inference
a) Total 4 peaks are present	4 types of proton present in the structure.
b) 2 peaks are present in the region 6.5 - 8.5 ppm	Aromatic ring is present

III] ^{13}C NMR Spectroscopy

Observation	Inference
a) Total 7 peaks are present	7 types of carbon atom is present.
b) 4 peaks are present in region 100 - 170 ppm	Aromatic ring is present

IV] UV Spectroscopy

Observation	Inference
a) There are 2 peaks in UV spectrum about 220nm	Compound is conjugate

Teacher's Sign :

EXPERIMENT : No.

II] ¹H NMR spectrum

Observation	Inference
a) Total 4 peaks are present	Total 4 type of proton present
b) 2 peaks at 6.5 - 8.5 ppm	Aromatic ring present.
c) There are 2 doublets in aromatic region.	Para - disubstituted aromatic ring present.
d) Singlet peak at 3.9 ppm	Due to CH_3 adjacent to O
e) Singlet peak at 2.5 ppm	Due to CH_3 at aromatic.

III] ¹³C NMR spectrum

Observation	Inference
a) Total 7 peaks are present	7 type of carbon is present
b) 4 peaks are present in region 100-170 ppm	Aromatic ring is present
c) Signal at 169 ppm	Due to ester carbon atom
d) There are 4 peaks in aromatic region i.e. 100-170 ppm	Para disubstituted benzene ring present
e) Out of 4 aromatic signal, 2 are missing in DEPT 135	2 quaternary C-atom present in aromatic ring.
f) Signal at 79 ppm in proton decoupled spectrum.	Due to solvent.
g) Signal at 52 ppm in DEPT 135	Due to CH_3 adjacent to O
h) Signal at 22 ppm in DEPT 135	Due to CH_3 at aromatic

IV] UV Spectrum

Observation	Inference
a) 2 peak in UV at 220 nm	Compound is conjugate
b) λ_{max} 238 nm ($\log_{10} \varepsilon$ 4.2)	Due to $\pi \rightarrow \pi^*$ transition
c) λ_{max} 281 nm ($\log_{10} \varepsilon$ 2.7)	Due to $n \rightarrow \pi^*$ transition.

V] Mass Spectrum

Observation	Inference
a) Molecular ion peak $M^{+\cdot}$	m/e = 150
b) Base peak	m/e = 119

B] Determination of molecular formula

Rule of 13 : $\frac{M}{13} = n + r$

No. of carbon $= \frac{M}{13} = \frac{150}{13} = 11$

No. of hydrogen $= M - (C \times 12) = 150 - (11 \times 12)$
$= 150 - 132 = 18$

∴ Base formula : $C_nH_{n+r} = C_{11}H_{11+7} = C_{11}H_{18}$

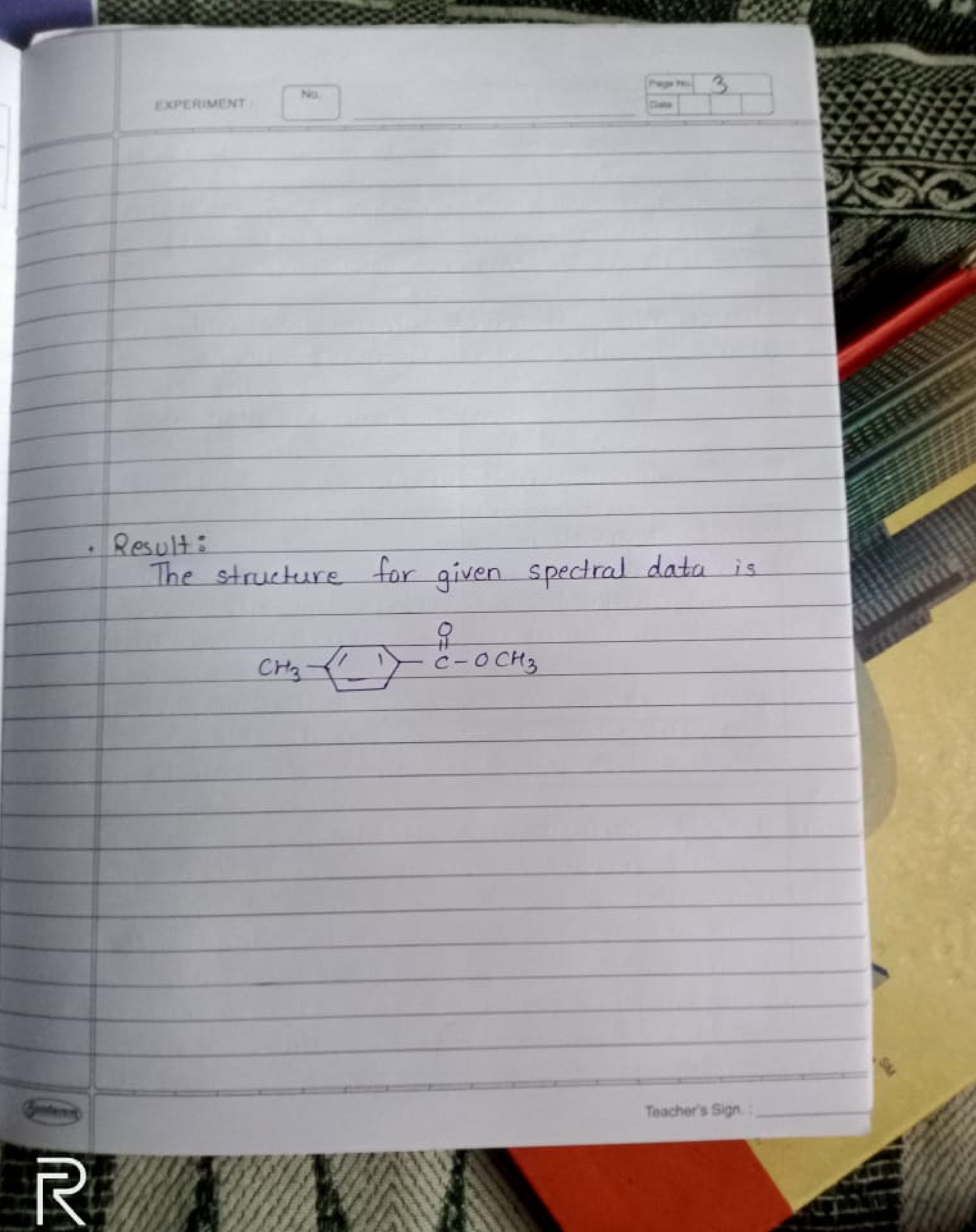
Molecular formula	Add element	Reason of adding	Substract equivalent	Modified formula	IHD
$C_{11}H_{18}$	-	-	-	$C_{11}H_{18}$	3
$C_{11}H_{18}$	O	Carbonyl group	CH_4	$C_{10}H_{14}O$	4
$C_{10}H_{14}O$	O	IHD is insufficient	CH_4	$C_9H_{10}O_2$	5

∴ Molecular formula is $C_9H_{10}O_2$

C] Detail Observation

I] IR spectrum

Observation	Inference
a) Strong observation at 1724 cm^{-1}	C=O stretching i.e. carbonyl group is present.
b) Medium observation at region 3100-2900 cm^{-1}	C-H stretching alkyl (sp^3) present.
c) Peak at 1600-1610 cm^{-1}	C=C stretching, aromatic ring is present.
d) Strong observation near 1100-1300 cm^{-1}	C-O stretching is present



EXPERIMENT :
No.
Page No. 3
Date
• Result :
The structure for given spectral data is
CH_3 — C₆H₄ — C(=O) — OCH_3
Teacher's Sign. :
Shot on realme U1

- Spectral identification No :- 2

A] preliminary observation

I] IR spectroscopy :-

Observation	Inference
a) strong observation at 1718 cm^{-1}	carbonyl group present.
b) Medium observation at 3000 cm^{-1}	Alcohol group may be present.

II] ^1H NMR Spectroscopy

Observation	Inference
a) Total 3 peaks are observed	3 types of protons are present.
b) There is no peak region to 6.5 - 8.5 ppm	This is an aliphatic compound.

III] ^{13}C NMR spectroscopy

Observation	Inference
a) Total 4 peaks are observed	4 types of carbon are present.
b) Peak at 210 ppm	carbonyl carbon is present

IV] UV spectroscopy :-

observation	Inference
a) peak at 265 nm	so compound is conjugated.

V] mass spectrum

observation	Inference
a) molecular ion peak $M^{+\cdot}$	m/e = 72
b) Base peak	m/e = 43

Teacher's Sign. :

B] Determination of Molecular formula :-

* Rule of 13 :- $\frac{M}{13} = n + r$

No. of carbon $\frac{M}{13} = \frac{72}{13} = 5$

No. of Hydrogen $M - (C \times 12)$
$= 72 - (5 \times 12)$
$= 72 - 60$
$= 12$

∴ Base formula $= C_nH_{n+r} = C_5H_{5+7} = C_5H_{12}$

Molecular formula	Add Element	Reason of Adding	Substract equivalent	Modified molecular formula	IHD
C_5H_{12}	–	–	–	C_5H_{12}	$x + y - \frac{y}{2}$ $5 + 1 - \frac{12}{2}$ $6 - 6$ $= 0$
C_5H_{12}	O	Carbonyl group	CH_4	C_4H_8O	$x + 1 - \frac{y}{2}$ $4 + 1 - \frac{8}{2}$ $5 - 4$ $= 1$

∴ Molecular formula : C_4H_8O

C] Detail observation :-

I] IR Spectrum -

Observation	Inference
a) strong observation at 1718 cm^{-1}	carbonyl group so acid, ketone may be present.
b) medium observation at 3000 cm^{-1}	C-H stretching alkyl (sp^3) present.
c) Peak at 1100 - 1200 cm^{-1}.	C-O stretching ester or acid, ketone or aldehyde may be present.

EXPERIMENT : No.   Page No. 5   Date

II] ^1H NMR spectrum :-

Observation	Inference
a) Total 3 peaks are observed	3 type of hydrogen are present
b) There is no peak region 6.5 to 8.5 ppm.	This is an aliphatic compound present.
c) peak at 2.4 ppm shows quadret	So - CH_2 is adjescent to - CH_3
d) peak at 2 ppm shows singlet	So - CH_3 is adjescent to carbonyl carbon.
e) Triplet peak at 0.8 ppm	So - CH_3 is adjescent to - CH_2

III] ^{13}C NMR Spectrum

observation	Inference
a) Total 4 peaks are observed	4 type of carbon is present
b) Peak at 210 ppm.	carbonyl carbon present
c) peak at region 30-40 ppm.	Due to CH_2 group
d) peak at region 20-30 ppm.	Due to -C group
e) peak at region 0-10 ppm	Due to - CH_3 group
f) singnal at 79 ppm in proton decoupled spectrum	Due to solvent.

IV] UV Spectrum -

a) Peak at 265 nm	so compound is conjugate because $\pi \rightarrow \pi^*$ transition

V] Mass Spectrum -

a) molecular ion peak $M^{+\cdot}$	m/e =
b) Base peak	m/e =

Teacher's Sign. : ___________

Sundaram

V] Mass spectrum :-

Observation	Inference
a) Molecular ion peak $M^{+\cdot}$	m/e = 192
b) Base peak	m/e = 135

- Determination of molecular formula :-
- Rule of 13 :- $\frac{M}{13} = n + r$

no. of carbon = $\frac{M}{13} = \frac{192}{13} = 14$

no. of Hydrogen = $M - (C \times 12) = 192 - (14 \times 12)$
$= 192 - 162$
$= 24$

∴ Base formula = $C_nH_{n+r} = C_{14}H_{14+10} = C_{14}H_{14+10} = C_{14}H_{24}$

Molecular Formula	Add Element	Reason of adding	Substract equivalent	Modified molecular formula	IHD
$C_{14}H_{24}$	–	–	–	$C_{14}H_{24}$	$n - 1 = y/2$ $= 14 + 1 = 24/2$ $= 15 - 12$ $= 3$
$C_{14}H_{24}$	O	carbonyl group	CH_4	$C_{13}H_{20}O$	9
$C_{13}H_{26}O$	O	IHD is insufficient	CH_4	$C_{12}H_{16}O_2$	5

∴ Molecular formula = $C_{12}H_{16}O_2$

- Detail observation :-

I) IR spectrum :-

Observation	Inference
a) Peak at 1766 cm^{-1}	C=O Stretching carbonyl grp present
b) Strong observation at 3000 cm^{-1}	C-H Stretching alkyl (csp^3) present
c) Peak at 1500 – 1600 cm^{-1}	C=C stretching, benzene present
d) Peak at 1200 - 1300 cm^{-1}	C-O stretching, ether, ester acid present.
e) Peak at 120 cm^{-1}	C-H Stretching para subsituted.

II] ^1H NMR Spectrum :-

Observation	Inference
a) There are 6 peaks observed	6 type of hydrogen present
b) 2 peaks present at 6.5-8.5 ppm.	Aromatic ring is present
c) Signal at region 2-2.5 ppm	so - CH_3 is due to aromatic ring
d) Signal at region 1-1.5 ppm	so - CH_3 is present.
e) There are doublet in region 6.5 - 8.5 ppm.	so it is para disubsituted aromatic ring present

III] ^{13}C NMR spectrum

Observation	Inference
a) There are 8 peaks present	8 type of carbons present
b) peak at 110-160 ppm	Aromatic ring is present
c) peak at range 160-180 ppm.	C-O stretching acid, ester, amide is present.
d) Peak at region 30-40 ppm	Arene C-Ar. present
e) peak at 77 ppm	Due to solvent
f) peak at 150 ppm	C=C stretching alkene is present
g) peak at region 20-30 ppm.	C=O stretching Acid, ester, amide is present.

IV] UV Spectrum :-

Observation	Inference
a) 2 Peak at about 260 - 270 nm	compound is conjugated
b) Peak at λmax 262 nm ($\log_{10} \varepsilon$ 2.6)	Due to $\pi \rightarrow \pi^*$ transition
c)	

Teacher's Sign. :

Sundaram

Spectral identification No :- 3

A] preliminary observation -

I] IR - spectroscopy -

	observation	Inference
a)	strong observation at 1766 cm^{-1}	C=O. stretching carbonyl group is present.
b)	strong observation at 3000 cm^{-1}	C-H stretching alkyl (sp^3) present.

II] ^1H NMR Spectroscopy

	observation	Inference
a)	There are 4 peaks are observed	Total 4 type of proton are present.
b)	2 peaks present at region 6.5 - 8.5 ppm.	Aromatic ring may be present

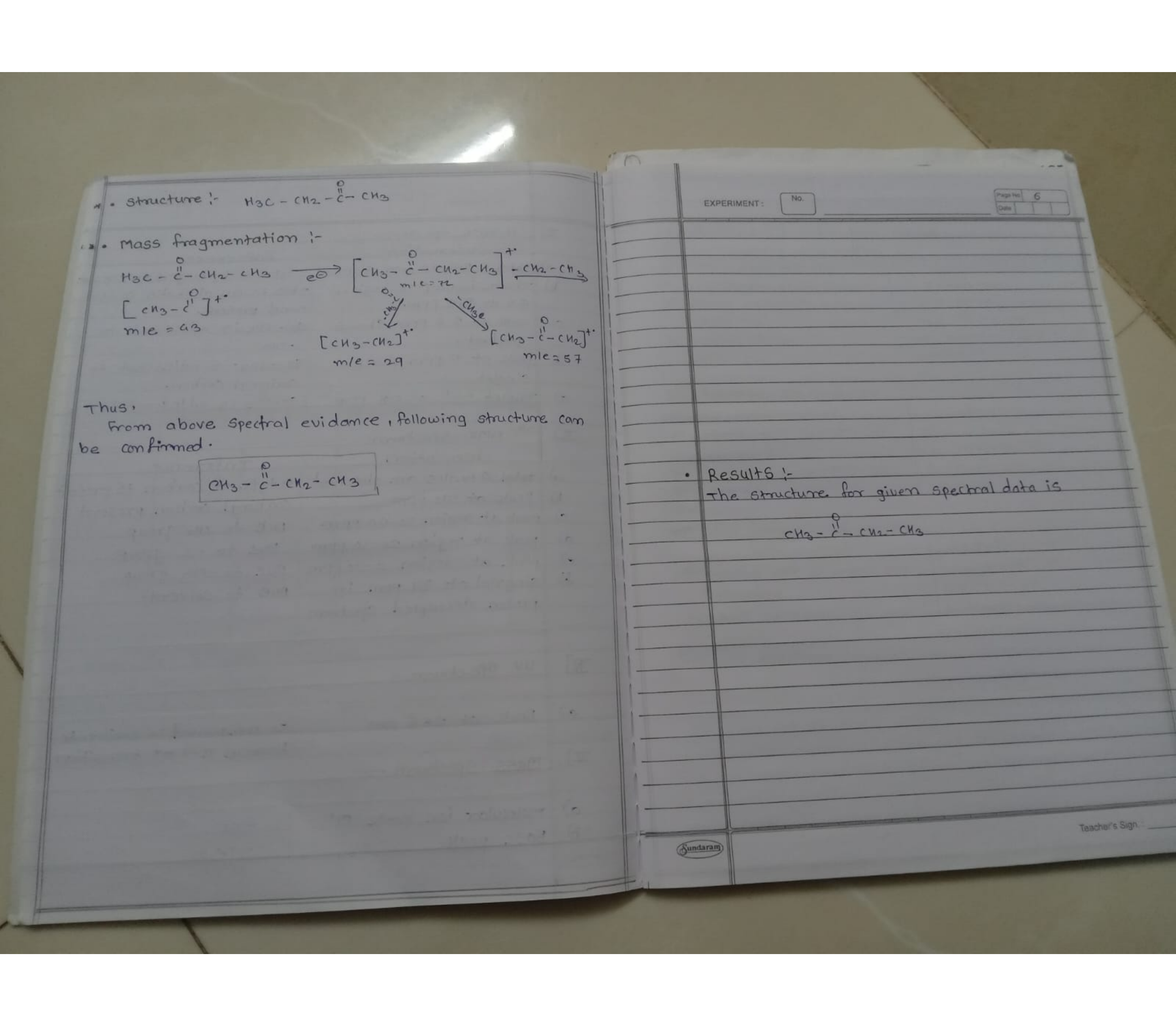
III] ^{13}C NMR spectroscopy

	observation	Inference
a)	There are 8 peaks are observed	Total 8 type of carbon are present.
b)	peak at range 110-160 ppm.	Aromatic ring may be present.

IV] UV spectrum :-

	observation	Inference
a)	peak at 262 nm & 269 nm	compound may be conjugated.

Teacher's Sign. :



• Structure :- $H_3C - CH_2 - \overset{O}{\overset{\|}{C}} - CH_3$

• Mass fragmentation :-

$H_3C - \overset{O}{\overset{\|}{C}} - CH_2 - CH_3 \xrightarrow{e^{\ominus}} [CH_3 - \overset{O}{\overset{\|}{C}} - CH_2 - CH_3]^{+\cdot}$ m/e = 72 $\xrightarrow{-CH_2-CH_3}$ $[CH_3 - \overset{O}{\overset{\|}{C}}]^{+\cdot}$ m/e = 43

$\xrightarrow{-\overset{O}{\overset{\|}{C}}-CH_3}$ $[CH_3 - CH_2]^{+\cdot}$ m/e = 29

$\xrightarrow{-CH_3}$ $[CH_3 - \overset{O}{\overset{\|}{C}} - CH_2]^{+\cdot}$ m/e = 57

Thus,
From above spectral evidance, following structure can be confirmed.

$CH_3 - \overset{O}{\overset{\|}{C}} - CH_2 - CH_3$

EXPERIMENT : No. Page No. 6 Date

• Results :-
The structure for given spectral data is

$CH_3 - \overset{O}{\overset{\|}{C}} - CH_2 - CH_3$

Teacher's Sign. :

Sundaram

Spectral identification No:- 9

A] preliminary observation

I] IR spectroscopy

Observation	Inference
a) strong observation at 1690 cm^{-1}	C=O carbonyl group is present.
b) Medium observation at 1300 - 1200 cm^{-1}	C-O stretching alcohol, ether may be present.

II] ^1H NMR spectroscopy -

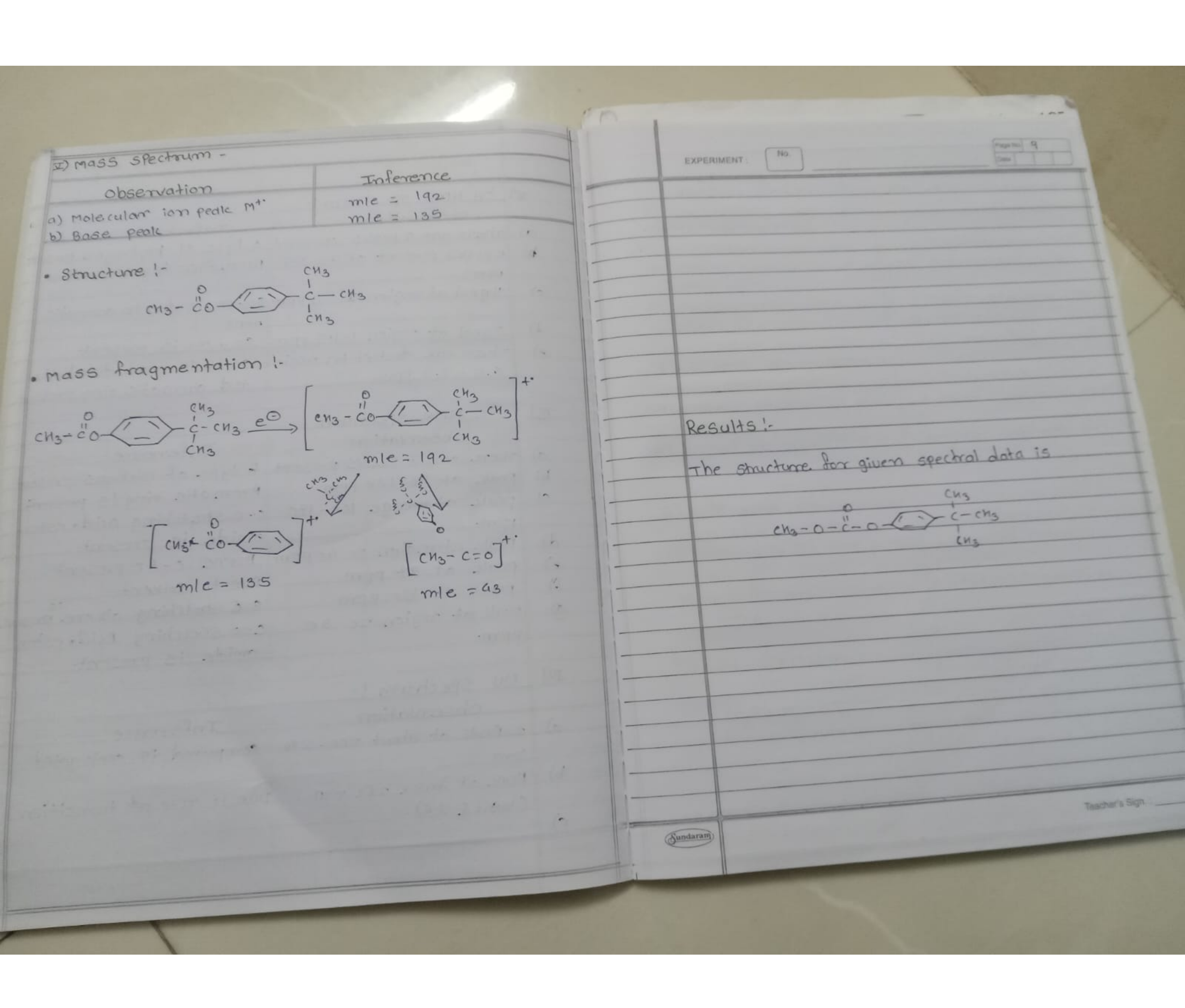
observation	Inference
a) Total 3 peaks are present.	3 type of proton is present.
b) signal at region 7-8 ppm.	Aromatic ring may be present.

III] ^{13}C NMR spectroscopy -

observation	Inference
a) Total 6 peaks are present.	6 type of carbon is present.
b) 4 peaks are present at region 120-160.	Aromatic ring may be present.

IV] UV spectrum :-

observation	Inference
a) peaks at 255 nm	compound may be conjugated.



V) Mass Spectrum -
Observation
Inference
a) Molecular ion peak $M^{+\cdot}$
m/e = 192
b) Base peak
m/e = 135
• Structure :-
$CH_3-CO-C_6H_4-C(CH_3)_3$
• Mass fragmentation :-
e⊖
m/e = 192
m/e = 135
$[CH_3-C=O]^{+\cdot}$
m/e = 43
EXPERIMENT
No.
Results :-
The structure for given spectral data is
Teacher's Sign
Sundaram

II) Mass spectrum :-

Observation	Inference
a) Molecular ion peak $M^{+\cdot}$	m/e = 154/156
b) Base peak	m/e = 139/141

B] Determination of molecular formula :-

Rule of 13 :- $\frac{M}{13} = n + r$

No. of carbon $\frac{M}{13} = \frac{154}{13} = 11$

No. of Hydrogen $M - C(C \times 12) = 154 - (11 \times 12)$
$= 154 - 132$
$= 22$

Base formula = C_nH_{n+r} = $C_{11}H_{11+11}$ = $C_{11}H_{22}$

Molecular formula	Add Element	Reason of Adding	Substract equivalent	Modified molecular formula	IHD
$C_{11}H_{22}$	-	-	-	-	1
$C_{11}H_{22}$	O	Carbonyl group	CH_4	$C_{10}H_{18}O$	2
$C_{10}H_{18}O$	O	present in mass spectra	C_2H_{11}	$C_8H_7O.Cl$	5

Molecular formula = C_8H_7OCl

- Detail observation –

I] IR Spectrum –

Observation	Inference
a) strong observation at 1690 cm^{-1}	C=O carbonyl group is present
b) medium observation at 1300 - 1200 cm^{-1}	C=O stretching alcohol, ether may be present.
c) Peak at 1600 cm^{-1}	C=C stretching benzene present
d) Peak at 820 cm^{-1}	para subsituted C-H stretching

EXPERIMENT : No.

II] ^{1}H NMR Spectroscopy –

Observation	Inference
a) 3 peaks are observed	Total 3 type of hydrogen present
b) 2 peaks are present in region 7-8 ppm	Aromatic ring is present
c) singlet peak at 2.6 ppm	Due to $-CH_3$ attach to aromatic ring.

III] ^{13}C NMR Spectroscopy –

Observation	Inference
a) peak at range 180 - 200 ppm	ketone C=O stretching
b) 4 peak at range 120 - 160 ppm.	Aromatic ring is present
c) Peak at $-CH_3$ at 20-30 ppm	Due to $-CH_3$ attach to $-C=O$

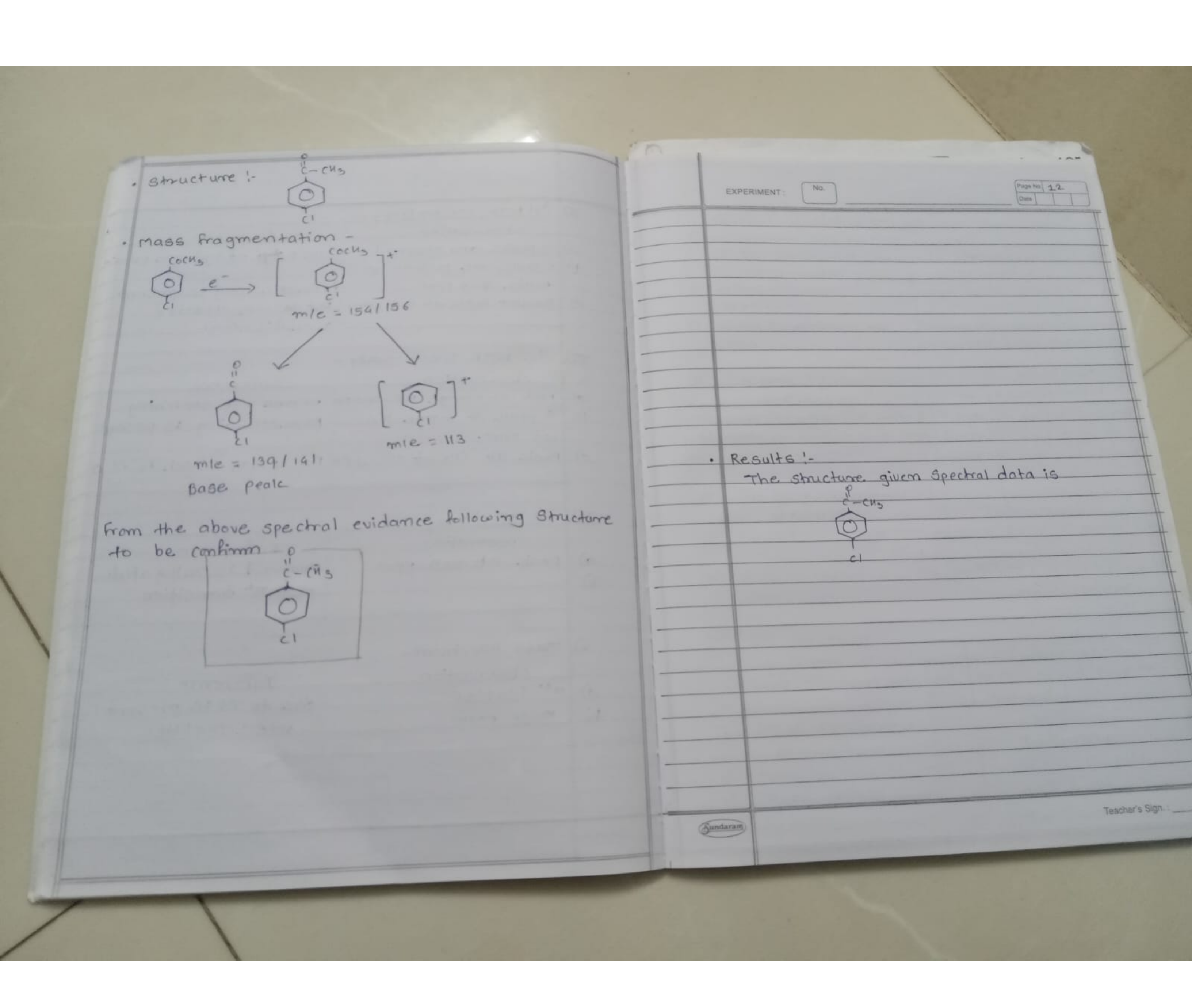
IV) UV spectrum –

Observation	Inference
a) peak at 225 ppm	compound is conjugated.
b)	$\pi \to \pi^*$ transition

V) Mass Spectrum –

Observation	Inference
a) $M^{+\cdot}$ 154/156	due to Cl is present
b) Base peak	m/e = 139/141

Teacher's Sign. :



• Structure :-

$C(=O)-CH_3$ on a benzene ring, with Cl in the para position

• Mass fragmentation -

$COCH_3$–C₆H₄–Cl $\xrightarrow{e^-}$ $[COCH_3$–C₆H₄–Cl$]^{+\cdot}$

m/e = 154/156

→ C(=O)–C₆H₄–Cl, m/e = 139/141, Base peak

→ $[$C₆H₄–Cl$]^+$, m/e = 113

From the above spectral evidance following Structure to be confirm

$C(=O)-CH_3$ on a benzene ring, with Cl in the para position

EXPERIMENT : No. Page No. 12 Date

• Results :-

The structure given Spectral data is

$C(=O)-CH_3$ on a benzene ring, with Cl in the para position

Teacher's Sign. :

- Spectral identification No - 5

A] preliminary observation -

I] IR spectroscopy -

observation	Inference
a) strong observation at 1773 cm^{-1}	carbonyl C=O stretching
b) strong observation at 1738 cm^{-1}	carbonyl C=O stretching carboxylic acid, ester present

II] ^{1}H NMR spectroscopy -

observation	Inference
a) Total 3 peaks are present	3 type of proton present
b) peak at region 7-8 ppm	Aromatic ring may be present.

III] ^{13}C NMR spectroscopy -

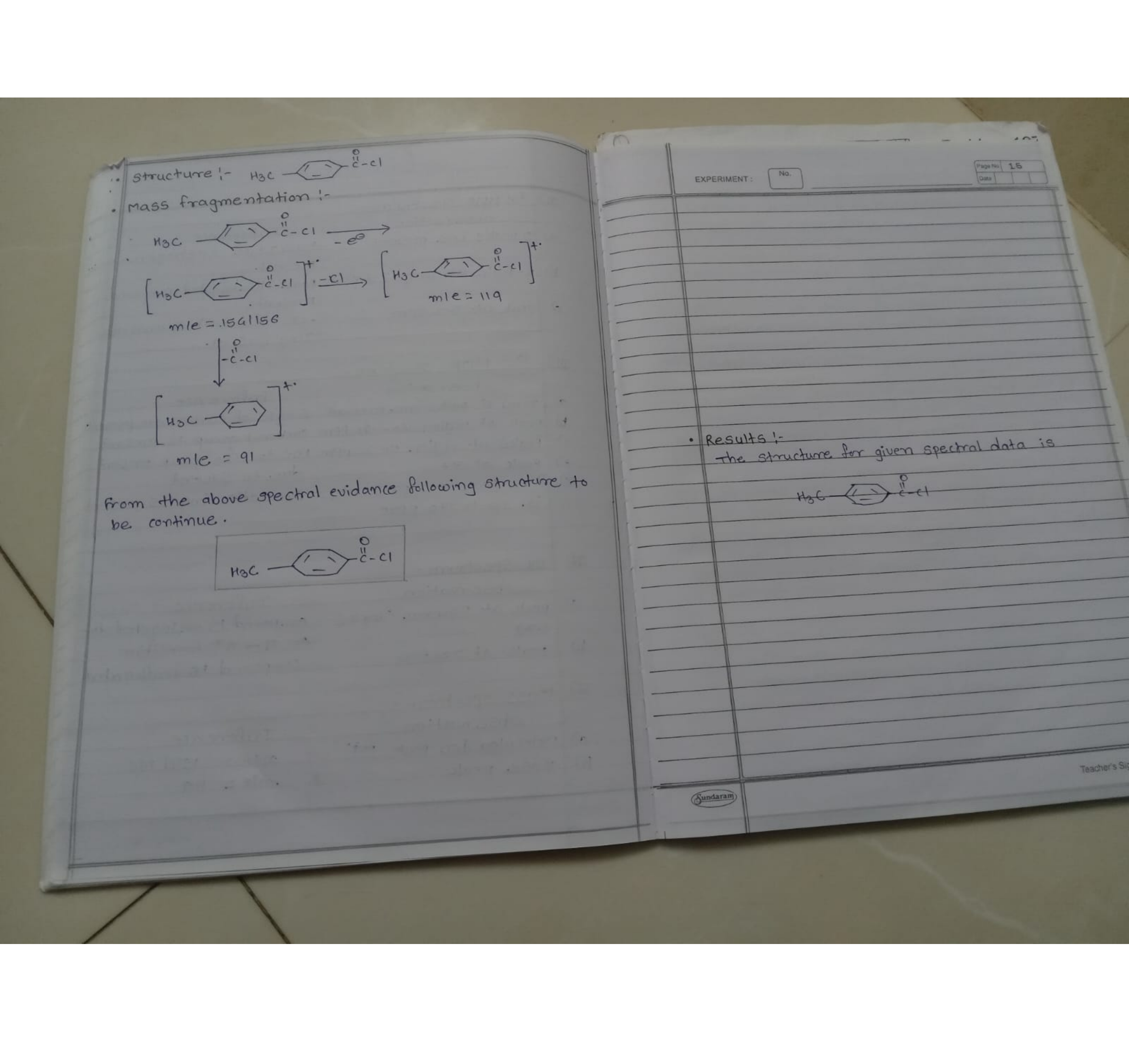
observation	Inference
a) Total 6 peaks are present	Total 6 type of carbon present.
b) peak at region 160-180 ppm.	carbonyl C=O stretching acid ester, amide present.

IV) UV spectrum -

observation	Inference
a) peak at about 220 nm	so compound may be conjugated

V] Mass spectrum -

observation	Inference
a) Molecular peak ion $M^{+\cdot}$	m/e = 154/156
b) Base peak	m/e = 119



- Structure :- H_3C – (benzene ring) – C(=O)–Cl
- Mass fragmentation :-

H_3C – (benzene ring) – C(=O)–Cl $\xrightarrow{-e^{\ominus}}$

$[H_3C$ – (benzene ring) – C(=O)–Cl$]^{+\cdot}$ $\xrightarrow{-Cl}$ $[H_3C$ – (benzene ring) – C(=O)$]^{+\cdot}$

m/e = 154/156   m/e = 119

↓ −C(=O)–Cl

$[H_3C$ – (benzene ring)$]^{+\cdot}$

m/e = 91

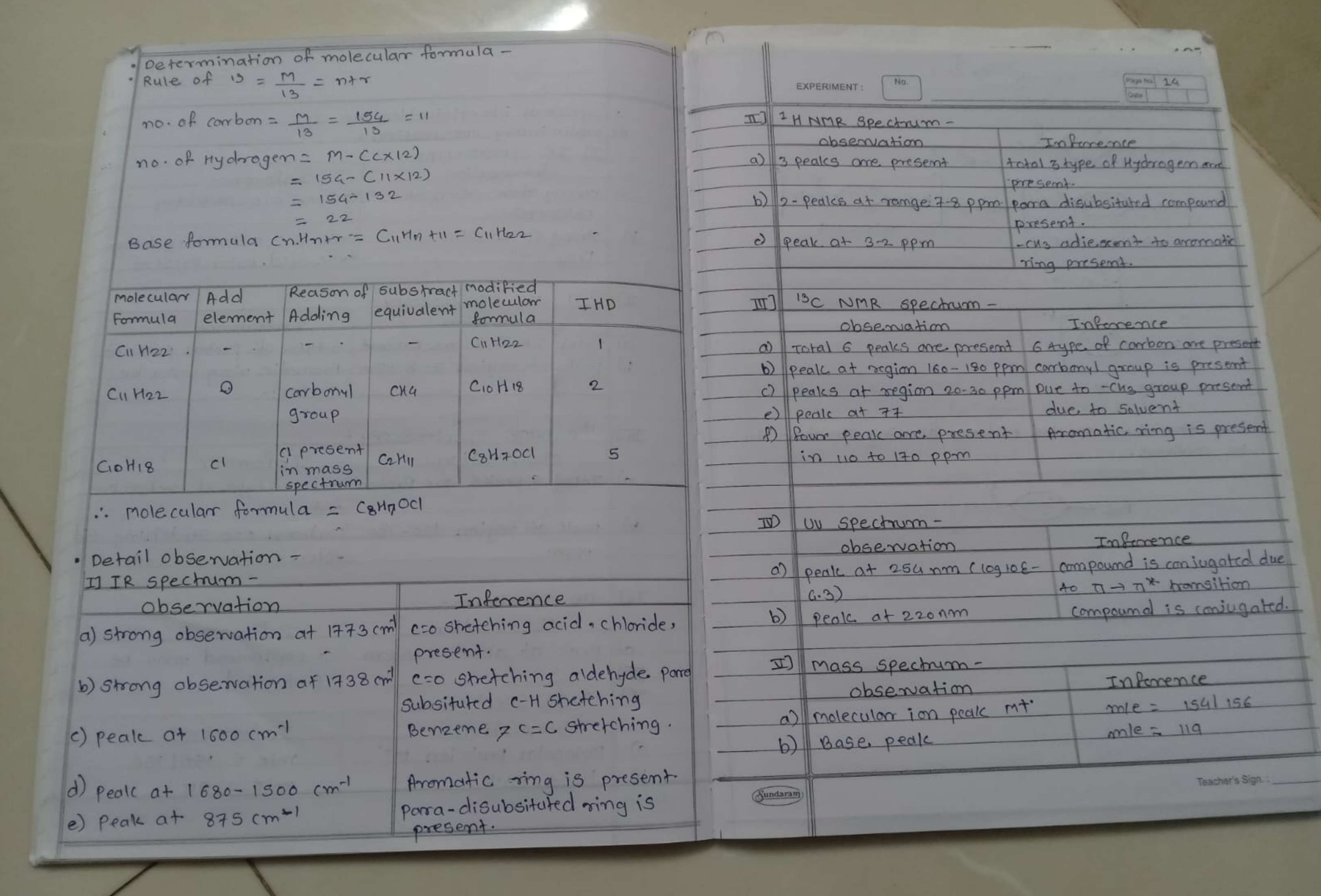
From the above spectral evidance following structure to be continue.

H_3C – (benzene ring) – C(=O)–Cl

EXPERIMENT :   No.   Page No. 15   Date

- Results :-
  The structure for given spectral data is

H_3C – (benzene ring) – C(=O)–Cl



- Determination of molecular formula –
- Rule of 13 = $\frac{M}{13} = n + r$

no. of carbon = $\frac{M}{13} = \frac{154}{13} = 11$

no. of Hydrogen = $M - (C \times 12)$
= $154 - (11 \times 12)$
= $154 - 132$
= 22

Base formula $C_nH_{n+r} = C_{11}H_{n+11} = C_{11}H_{22}$

Molecular Formula	Add element	Reason of Adding	Substract equivalent	Modified molecular formula	IHD
$C_{11}H_{22}$	–	–	–	$C_{11}H_{22}$	1
$C_{11}H_{22}$	O	carbonyl group	CH_4	$C_{10}H_{18}$	2
$C_{10}H_{18}$	Cl	Cl present in mass spectrum	C_2H_{11}	C_8H_7OCl	5

∴ Molecular formula = C_8H_7OCl

- Detail observation –

I] IR Spectrum –

Observation	Inference
a) strong observation at 1773 cm^{-1}	C=O stretching acid. chloride, present.
b) strong observation at 1738 cm^{-1}	C=O stretching aldehyde. Para subsituted C-H stretching
c) peak at 1600 cm^{-1}	Benzene > C=C stretching.
d) peak at 1680-1500 cm^{-1}	Aromatic ring is present
e) peak at 875 cm^{-1}	Para-disubsituted ring is present.

EXPERIMENT: No. Page No. 14 Date

II] ^1H NMR Spectrum –

	Observation	Inference
a)	3 peaks are present	total 3 type of Hydrogen are present.
b)	2-peaks at range 7-8 ppm	para disubsituted compound present.
c)	peak at 3-2 ppm	$-CH_3$ adjacent to aromatic ring present.

III] ^{13}C NMR spectrum –

	Observation	Inference
a)	Total 6 peaks are present	6 type of carbon are present
b)	peak at region 160-180 ppm	carbonyl group is present
c)	peaks at region 20-30 ppm	Due to $-CH_3$ group present
e)	peak at 77	due to solvent
f)	four peak are present in 110 to 170 ppm	Aromatic ring is present

IV) UV spectrum –

	Observation	Inference
a)	peak at 254 nm ($\log_{10}\varepsilon$ – 4.3)	compound is conjugated due to $\pi \rightarrow \pi^*$ transition
b)	peak at 220 nm	compound is conjugated.

V) Mass spectrum –

	Observation	Inference
a)	molecular ion peak $M^{+\cdot}$	m/e = 154/156
b)	Base peak	m/e = 119

Sundaram

Teacher's Sign.:

- spectral identification No - 6

A] prilimінary observation -

I] IR - spectroscopy -

observation	Inference
a) observation at 1693 cm^{-1}	c=o stretching aldehyde, ketone may be present.
b) observation at 1600 cm^{-1}	c=o stretching. benzene may be present

II] ^{1}H NMR Spectroscopy -

observation	Inference
a) 3 peaks are observed	Total 3 peaks types of proton are present
b) Two peaks present in region 7-8 ppm.	Aromatic ring may be present.

III] ^{13}C NMR spectroscopy -

observation	Inference
a) Total 6 peaks are observed.	Total 6 types of carbon are present.
b) peak present at region 110-160 ppm.	Aromatic ring may be present.

IV] UV spectrum -

observation	Inference
a) peak at above 220 nm	compound may be conjugated.

V] Mass Spectrum -

Observation	Inference
a) molecular ion peak $m^{+\cdot}$	m/e = 198/200
b) Base peak	m/e = 183/185

• Determination of molecular formula -

Rule of 13 = $\frac{M}{13} = n + \frac{r}{13}$

no. of carbon = $\frac{M}{13} = \frac{198}{13} = 15$

no. of Hydrogen = $M - (C \times 12) = 198 - (15 \times 12)$
$= 198 - 180 = 18$

∴ Base formula = $C_nH_{n+r} = C_{15}H_{15+3} = C_{15}H_{18}$

Molecular formula	Add element	Reason of adding	Substract equivalent	Modified molecular formula	IHD
$C_{15}H_{18}$	–	–	–	$C_{15}H_{18}$	7
$C_{15}H_{18}$	O	carbonyl group	CH_4	$C_{14}H_{14}O$	8
$C_{14}H_{14}O$	Br	Br present in mass spectrum	C_6H_7	C_8H_7OBr	5

∴ molecular formula = C_8H_7OBr

• Detail observation -

I] IR Spectrum -

Observation	Inference
a) strong observation at 1963 cm^{-1}	C=O stretching ketone or aldehyde present.
b) medium observation at 1600 cm^{-1}	C=C stretching benzene present
c) peak at region 1200-1300 cm^{-1}	C=O stretching ketone, aldehyde present.
d) observe at peak 3000-2900 cm^{-1}	C-H stretching of sp^3 carbon present.

II] ^1H NMR spectroscopy -

Observation	Inference
a) 3 peaks are present	3 type of hydrogen present
b) 2 peaks at region 7-8 ppm	aromatic ring present
c) Two peak doublet at region 7-8 ppm.	para-disubstituted aromatic ring present.
d) singlet at 2-3 ppm	Due to $-CH_3$ at aromatic ring present.

III] ^{13}C NMR spectroscopy -

Observation	Inference
a) peak at region 160-200 ppm.	C=O group is present
b) 4 peak at region 120-160 ppm	Aromatic ring is present
c) peak at 20-50 ppm	Due to $-CH_3$ at aromatic ring
d) peak at 77 ppm	Due to solvent

IV] UV spectrum -

Observation	Inference
a) peak at 257 nm ($\log \varepsilon$ 4.2)	compound is conjugate.
b) peak at above 220 nm	compound may be conjugate

V] Mass spectrum -

Observation	Inference
a) molecular peak ion $m^{+\cdot}$	m/e = 198/200
b) Base peak	m/e = 183/185

- Spectral identification No - 7
- preliminary observation -

I] IR spectroscopy -

	observation	Inference
a)	strong peak at region 1760 cm^{-1}	c=o stretching ketone & aldehyde may be present.
b)	medium peak at region 3000 - 2900 cm^{-1}	c-H stretching alkane may be present.

II] ^{1}H NMR Spectroscopy -

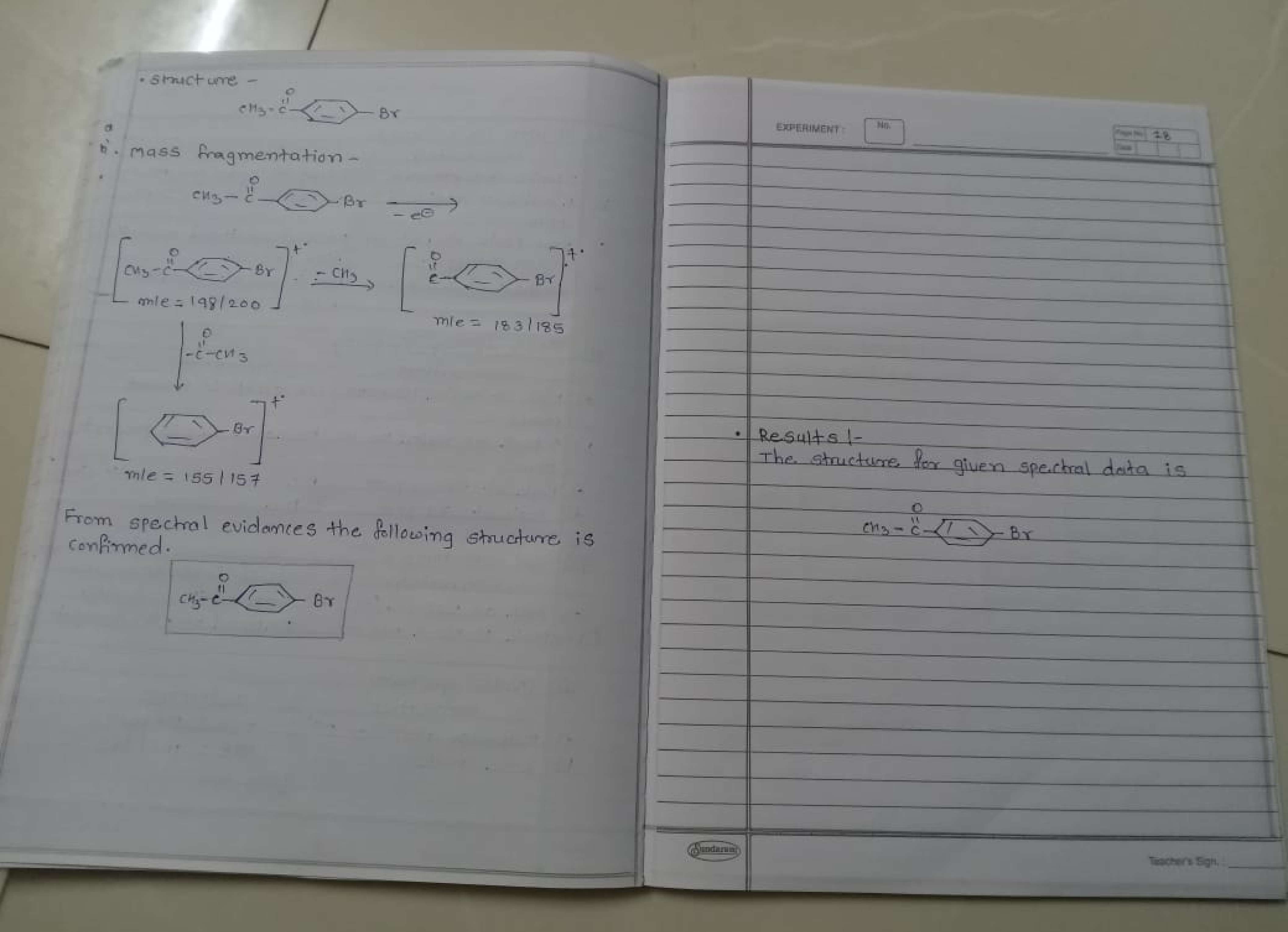
	observation	Inference
a)	There are 4 peaks are observed	Total four type of proton are present.
b)	Two peaks at region 6.5 - 8.5 δ ppm	Aromatic ring may be present.

III] ^{13}C NMR spectroscopy -

	observation	Inference
a)	There are 6 peaks are observed.	Total 6 type of carbon are present
b)	peak observe at 160 - 190 ppm.	carbonyl group may be present.

IV] UV spectrum -

	observation	Inference
a)	peak at above 220 nm	compound may be conjugated



• Structure -
$CH_3-C(=O)-C_6H_4-Br$
b. mass fragmentation -
$CH_3-C(=O)-C_6H_4-Br \xrightarrow{-e^{\ominus}}$
$[CH_3-C(=O)-C_6H_4-Br]^{+\cdot}$ m/e = 198/200 $\xrightarrow{-CH_3}$ $[C(=O)-C_6H_4-Br]^{+\cdot}$ m/e = 183/185
$-C(=O)-CH_3$
$[C_6H_4-Br]^{+\cdot}$ m/e = 155/157
From spectral evidances the following structure is confirmed.
$CH_3-C(=O)-C_6H_4-Br$
EXPERIMENT : No.
Page No. 28
Date
• Results :-
The structure for given spectral data is
$CH_3-C(=O)-C_6H_4-Br$
Sundaram
Teacher's Sign.

- Structure :-

$H_3C-\overset{O}{\overset{\|}{C}}-O-C_6H_4-CH_3$

- Mass fragmentation :-

$H_3C-\overset{O}{\overset{\|}{C}}-O-C_6H_4-CH_3 \xrightarrow{-e^{\ominus}}$

$\left[H_3C-\overset{O}{\overset{\|}{C}}-C_6H_4-CH_3\right]^{+\cdot} \xrightarrow{-CH_3\overset{O}{\overset{\|}{C}}} \left[C_6H_5-CH_3\right]^{+\cdot}$

m/e = 150   m/e = 108

From spectral evidamce the following structure is confirmed

$H_3C-\overset{O}{\overset{\|}{C}}-O-C_6H_4-CH_3$

- Results :-

The formula for given spectral data is

$H_3C-\overset{O}{\overset{\|}{C}}-O-C_6H_4-CH_3$

V] Mass spectrum -

observation	Inference
a) molecular ion peak $M^{+\cdot}$	m/e = 150
b) Base peak.	m/e = 108

- Determination of molecular formula :-

Rule of 13 = $\frac{M}{13} = n + r$

no. of carbon = $\frac{M}{13} = \frac{150}{13} = 11$

no. of Hydrogen = $M - (C \times 12) = 150 - (11 \times 12)$
$= 150 - 132$
$= 18$

∴ Base formula $C_nH_{n+r} = C_{11}H_{11+7} = C_{11}H_{18}$

Molecular formula	Add element	Reason of adding	Subscrition equivalent	modified molecular formula	IHD
$C_{11}H_{18}$	-	-	-	$C_{11}H_{18}$	3
$C_{11}H_{18}$	O	carbonyl compound	CH_4	$C_{10}H_{14}$	4
$C_{10}H_{14}O$	O	IHD is insufficient	CH_4	$C_9H_{10}O_2$	5

∴ molecular formula = $C_9H_{10}O_2$

- Detail observation -

I] IR spectrum -

observation	Inference
a) observe at strong peak at 1760 cm^{-1}	C=O Stetching ketone, aldehyde, present.
b) medium peak at p 3000 - 2900 cm^{-1}	C-H Stretching alkane present
c) medium peak at 1500 cm^{-1}	C-O stetching ester ketone present.

II] ^{13}C NMR spectroscopy -

	observation	Inference
a)	Total 6 peaks are present	6 type of ~~hydrogen~~ carbon present
b)	peak at range 162 - 180 ppm	C=O stetching
c)	four peak at 120 - 160 ppm	Aromatic ring present
d)	peak at region 20-30 ppm	C=O stretching
e)	peak at ~~7~~ 77 ppm	Due to solvent

III] ^{1}H NMR spectroscopy -

	observation	Inference
a)	There are 4 peak present	4 type of hydrogen are present.
b)	2 peaks at region 7-7.5 ppm.	C=C Stetching benzene present
c)	Doublet peak at 7-8 ppm	para-disubsituted aromatic

IV] UV Spectrum -

	observation	Inference
a)	peak at 265 nm (log₁₀ε 2.6)	Due to $\pi \rightarrow \pi^*$ transition
b)	peak at above 220 nm	compound is conjugate

V] mass spectrum -

	observation	Inference
a)	Molecular ion peak $M^{+\cdot}$	m/e = 150
b)	Base peak	m/e = 108

- Spectral identification No - 8

A] Preliminary observation -

I] IR spectroscopy -

	Observation	Inference
a)	Strong peak at 3326 cm^{-1}	O-H stretching may be present.
b)	peak at 1085 cm^{-1}	C-O stretching may be present

II] $^{1}H^{1}$ NMR spectroscopy -

	Observation	Inference
a)	They are five peak are observed.	Total 5 peaks of type of proton.
b)	peak at region 6.5 - 8.5 ppm.	Aromatic ring may be present.

III] ^{13}CNMR spectroscopy -

	Observation	Inference
a)	There are 6 peaks are observed.	Total 6 type of carbon are present.
b)	Peak at 110-160 ppm	Aromatic ring may be present

IV] UV spectrum -

	Observation	Inference
a)	$\log_{10} \varepsilon = 3.4$ U.V Spectrum	due to $\pi \rightarrow \pi^{*}$ transition hydroxy group Present

V] Mass spectrum -

	Observation	Inference
a)	Molecular peak ion $M^{+\cdot}$	m/e = 138
b)	Base peak	m/e = 107

• Determination of molecular formula -
Rule of 13 = $\frac{M}{13}$ =

no. of carbon = $\frac{M}{13} = \frac{138}{13} = 10$

no. of Hydrogen = $M - (C \times 12)$
= $138 - (10 \times 12)$
= 18

∴ Base formula $C_nH_{n+r} = C_{10}H_{18+8}$

Molecular formula	Add Element	Reason of adding	Substract equivalent	Modified molecular formula	IHD
$C_{10}H_{18}$	–	–	–	$C_{10}H_{18}$	2
$C_{10}H_{18}$	O	carbonyl group	CH_4	C_9H_{14}	3
C_9H_{14}	O	Hydroxy group	CH_4	$C_8H_{10}O_2$	5

Molecular formula = $C_8H_{10}O_2$

• Detail observation -
I] IR - spectrum -

Observation	Inference
a) Strong peak at 3326 cm^{-1}	Ar - OH phenol present
b) Sharp peak at 1085 cm^{-1}	C-O Stretching ether group present.
c) Medium peak at region 3000 - 2900 cm^{-1}	CH (SP^3) stretching - CH_3 group is present
d) Medium peak at region 3100 - 3000 cm^{-1}	C-H stretching - CH_2 group is present.
e) medium peak at 1500 - 1600 cm^{-1}	C=C stretching benzene present.

II] 1H NMR Spectrum -

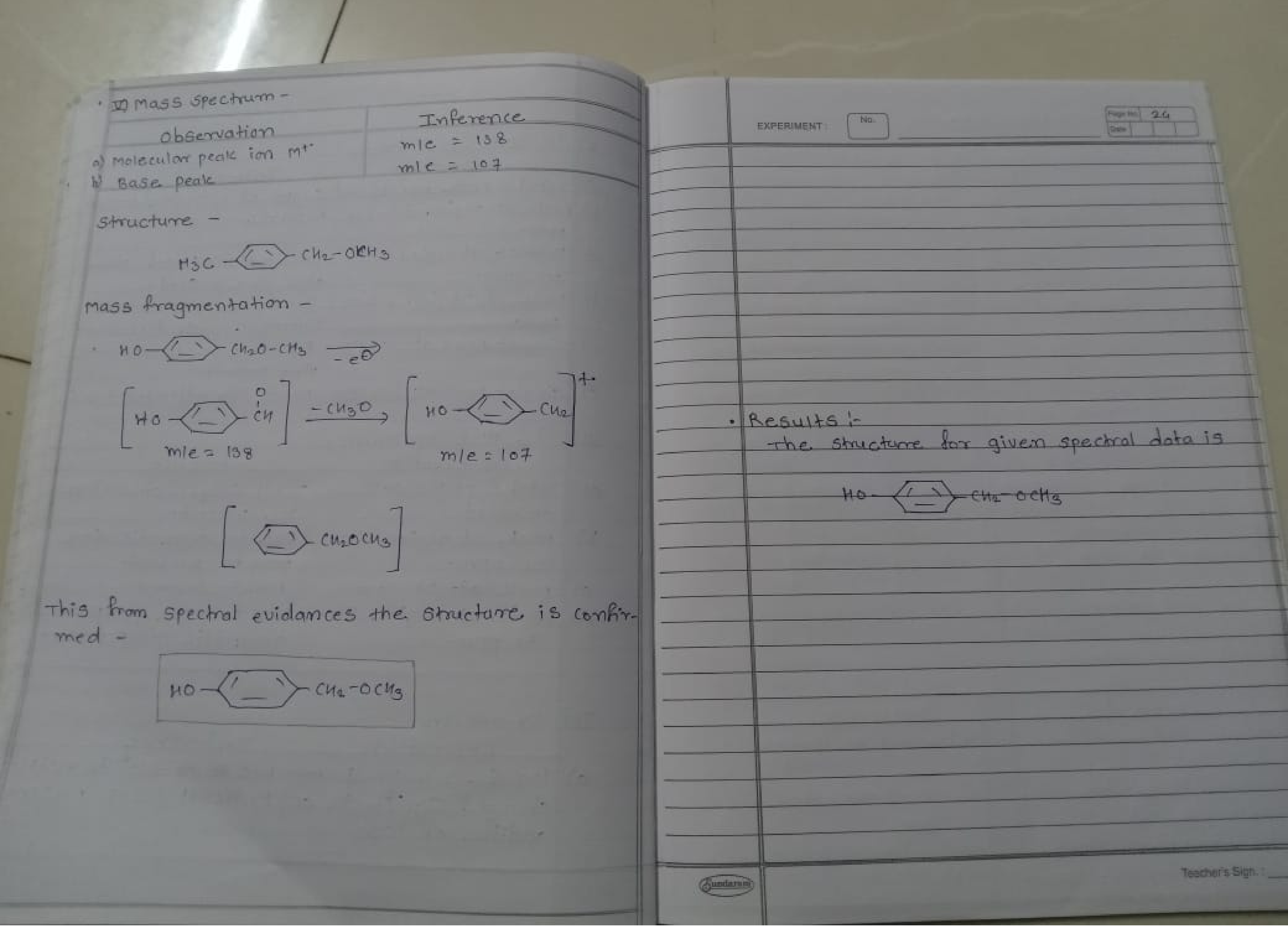
	Observation	Inference
a)	Total 5 peak are observed	5 type of hydrogen present
b)	peak at region 6.5 - 8.5 ppm.	Aromatic ring present.
c)	Doublet at region 6.5 - 8.5 ppm.	para - disubsituted aromatic ring present.
d)	peak at region 7.5 - 8.5 ppm.	Due to replacement of hydrogen with durterium
e)	singlet peak at 6.5 ppm	Due to - CH_2 to aromatic ring present.
f)	singlet peak at 3.4 ppm	Due to - CH_2 adjescent to O.

III] ^{13}C NMR Spectrum -

	Observation	Inference
a)	Total 6 peaks are observed.	Total 6 type of carbon are present.
b)	peak at region 110 - 150 ppm.	Due to aromatic ring may be present.
c)	peak at 77 ppm	Due to solvent
d)	peak at region 70 - 80 ppm.	Due to - CH_2 group to aromatic group present

IV] UV Spectrum -

	Observation	Inference
a)	log ε = 3.4 UV spectrum changed significantly on addition of base	Due to $\pi \rightarrow \pi^*$ transition Hydroxyl group present



• XI) Mass Spectrum -

Observation	Inference
a) molecular peak ion $M^{+\cdot}$	m/e = 138
b) Base peak	m/e = 107

Structure -

H_3C –(benzene ring)– CH_2-OCH_3

Mass fragmentation -

• HO –(benzene ring)– CH_2O-CH_3 $\xrightarrow{-e^{\ominus}}$

[HO –(benzene ring)– CH(=O)] m/e = 138 $\xrightarrow{-CH_3O}$ [HO –(benzene ring)– CH_2 $]^{+\cdot}$ m/e = 107

[(benzene ring)– CH_2OCH_3]

This from spectral evidances the structure is confirmed -

HO –(benzene ring)– CH_2-OCH_3

• Results :-
The structure for given spectral data is

HO –(benzene ring)– CH_2-OCH_3

• Spectral identification No - 9

A] preliminary observation -

I] IR - spectroscopy -

observation	Inference
a) Strong observation at 2209 cm^{-1}	C≡N group may be present
b) peak at 1500-1600 cm^{-1}	C=C stretching benzene may be present.

II] ^1H NMR Spectroscopy -

observation	Inference
a) There are 3 peaks observed	Total 3 types of hydrogen present
b) peak at 6.5 - 8.5	para - disubsituted aromatic ring present

III] ^{13}C NMR Spectroscopy -

observation	Inference
a) There 6 peaks are observed	Total 6 type of carbons are present.
b) peak at region 110-160 ppm.	Aromatic ring may be present.

IV] Mass Spectrum :-

observation	Inference
a) Molecular peak ion $M^{+\cdot}$	m/e = 146
b) Base peak	m/e = 145

- Determination of molecular formula -

Rule of 13 = $\frac{M}{13}$ = $n + r$

no. of carbon = $\frac{M}{13} = \frac{146}{13} = 11$

no. of hydrogen = $M - C(\times 12)$
= $146 - C(11 \times 12)$
= $146 - 132$
= 14

∴ Base formula = C_nH_{n+r} = $C_{11}H_{10+4}$ = $C_{11}H_{14}$

Molecular Formula	Add element	Reason of Adding	Substract equivalent	modified molecular formula	IHD
$C_{11}H_{14}$	-	-	-	$C_{11}H_{14}$	5
$C_{11}H_{14}$	N	Nitrile group	CH_2	$C_{10}H_{12}N$	5
$C_{10}H_{12}N$	N	IHD is insufficient	CH_2	$C_9H_{10}N_2$	6

- Detail observation -

I] IR Spectrum -

Observation	Inference
a) strong observation at 2209 cm^{-1}	C≡N may be present.
b) medium observation at 1600 - 1400 cm^{-1}	C=C stretching benzene is present.
c) peak at 800 - 900 cm^{-1}	para - disubsituted aromatic ring present.
d) strong peak at 3000 - 2900 cm^{-1}	C≡N Nitrile is present

II] ^1H NMR Spectrum -

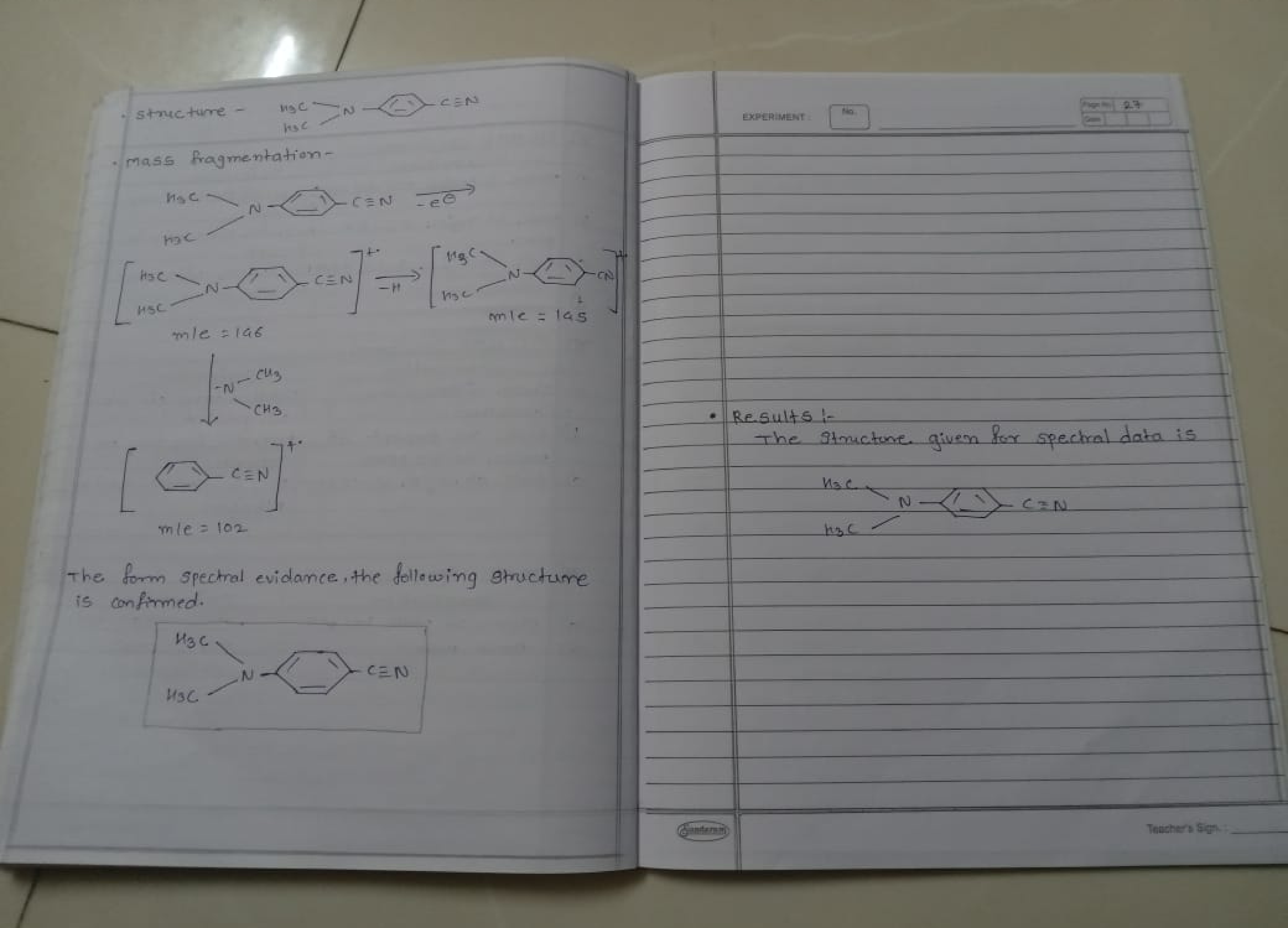
Observation	Inference
a) There 3 peaks are observ	3 type of protons are present
b) peak at region 6.5 - 8.5 ppm.	Aromatic ring may be present
c) peak at region 3 - 3.5 ppm	Due to $-CH_3$ adiescent to nitrogen.

III) ^{13}C NMR Spectrum -

Observation	Inference
a) There 6 peaks are observed	Total 6 type of carbon are present
b) peaks are present at region 110 - 160 ppm.	Aromatic ring may be present.
c) peak at region 35 - 40 ppm	Due to $-CH_3$ attached to Nitrogen

IV] Mass Spectrum -

Observation	Inference
a) Molecular peak ion M^{+}	m/e = 146
b) Base peak	m/e = 145



• structure - H_3C, H_3C – N – (benzene ring) – C≡N

• mass fragmentation -

H_3C, H_3C – N – (benzene ring) – C≡N $\xrightarrow{-e^{\ominus}}$

$[(H_3C)_2N–C_6H_4–C≡N]^{+\cdot}$ $\xrightarrow{-H}$ $[(H_3C)_2N–C_6H_3–CN]^{+}$

m/e = 146 m/e = 145

↓ $-N(CH_3)(CH_3)$

$[C_6H_5–C≡N]^{+\cdot}$

m/e = 102

The form spectral evidance, the following structure is confirmed.

H_3C, H_3C – N – (benzene ring) – C≡N

• Results :-

The structure given for spectral data is

H_3C, H_3C – N – (benzene ring) – C≡N

EXPERIMENT : No. 10 Page No. 28 Date

• Spectral identification NO- 10

A] preliminary observation-

I] IR spectroscopy

observation	Inference
a) strong observation at 3000 cm^{-1}	C-H stretching alkane may be present
b) medium observation at 1400 - 1500 cm^{-1}	C=C stretching benzene may be present

II] ^{1}H NMR spectroscopy-

observation	Inference
a) Two peaks are observed	Two type of protons are present.
b) peak at 6-8 ppm.	Aromatic ring may be present.

III] ^{13}C NMR spectroscopy-

observation	Inference
a) 4 peaks are observed.	4 types of carbon are present.
b) peak at 110-160 ppm.	Aromatic ring may be present.

IV] UV spectrum-

observation	Inference
a) Peak are about 220 nm	compound may be conjugated.

V) mass spectrum -

Observation	Inference
a) molecular peak ion	m/e = 182
b) Base peak	m/e = 91

- Determination of molecular formula -

Rule of 13 = $\frac{M}{13}$ = n+r

no. of carbon = $\frac{M}{13} = \frac{182}{13}$ = 14

no. of Hydrogen = M - (C×12)
= 182 - (14×12)
= 182 - 168
= 14

Base formula :- $C_nH_{n+r} = C_{14}H_{14+0} = C_{14}H_{14}$

IHD =

- Detail observation -

I] IR spectrum -

Observation	Inference
a) strong observation at 3000 cm^{-1}	C-H stretching alkane is present.
b) Medium observation at region 700 - 800 cm^{-1}	mono-substituted C-H stretching aromatic ring present
c) Peak at region 1600-1500 cm^{-1}	C=C stretching aromatic ring present.

II] ^1H NMR spectrum -

	Observation	Inference
a)	2 peaks are present	2 type of Hydrogen present.
b)	peak at 2.5-3ppm.	Due to $-CH_2$ aromatic ring
c)	peak at 7-8 ppm	Aromatic ring present

III] ^{13}C NMR spectrum

	Observation	Inference
a)	4 peaks are present	4 type of carbon present
b)	peak at region 110-160 ppm	Aromatic ring present
c)	peak at 30-40 ppm.	Due to $-CH_2$ group present

IV] UV Spectrum -

	Observation	Inference
a)	peak at above 220 nm	compound is conjugated.

V] mass spectrum

	Observation	Inference
a)	molecular peak ion M^{+}	m/e = 182
b)	Base peak	m/e = 91

V] Mass spectrum

Observation	Inference
a) Molecular ion peak $M^{+\cdot}$	m/e = 150
b) Base peak	m/e = 119

· Structure : $H_3C-C_6H_4-\overset{O}{\overset{\|}{C}}-OCH_3$

· Mass fragmentation :

$$H_3C-C_6H_4-\overset{O}{\overset{\|}{C}}-O-CH_3 \xrightarrow{e^{\ominus}} \left[H_3C-C_6H_4-\overset{O}{\overset{\|}{C}}-OCH_3\right]^{+\cdot}$$

m/e = 150

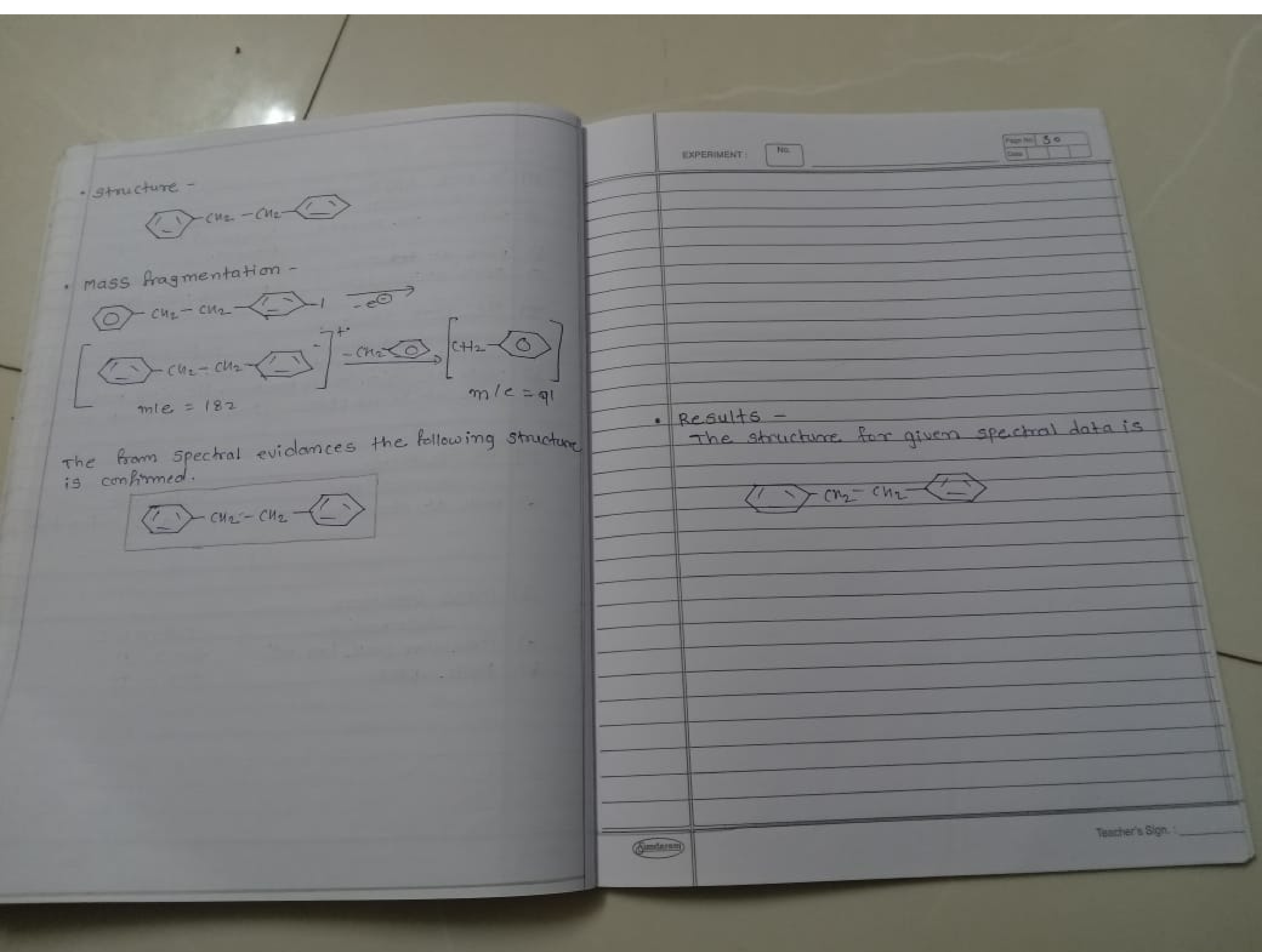
$-OCH_3$ → $\left[CH_3-C_6H_4-\overset{O}{\overset{\|}{C}}\right]^{\cdot +}$ m/e = 119

$-COOCH_3$ → $\left[CH_3-C_6H_4\right]^{+\cdot}$ m/e = 91

Thus, from above spectral evidence, the following structure can be confirmed.

$$CH_3-C_6H_4-\overset{O}{\overset{\|}{C}}-O-CH_3$$

Shot on realme U1



• structure -

$C_6H_5-CH_2-CH_2-C_6H_5$

• mass fragmentation -

$C_6H_5-CH_2-CH_2-C_6H_5 \xrightarrow{-e^-} [C_6H_5-CH_2-CH_2-C_6H_5]^{+\cdot} \xrightarrow{-CH_2C_6H_5} [CH_2-C_6H_5]^+$

m/e = 182

m/e = 91

The from spectral evidances the following structure is confirmed.

$C_6H_5-CH_2-CH_2-C_6H_5$

• Results -

The structure for given spectral data is

$C_6H_5-CH_2-CH_2-C_6H_5$